

## **Towards understanding of powder EPR spectra of irradiated sugars applied in dosimetry and detection of irradiated foodstuffs**

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Ionising radiation produces stable radicals in carbohydrates, like sugars, in concentrations correlated with the radiation dose. These radicals can be measured using electron paramagnetic resonance (EPR) spectroscopy, the intensity of the spectrum being indicative of the radiation dose [1]. In particular sucrose, the main component of table sugar, present in nearly every household and quite radiation-sensitive, is considered as an interesting dosimeter in case of radiation accidents with risk of public exposure. Sugar-containing foodstuffs usually contain a mixture of sugars, all exhibiting their distinct EPR signal with specific dose response, and overlapping in the total spectrum. Hence they can also be used to detect irradiation. The complexity of EPR spectra of radicals in sugars, as a result of many hyperfine interactions, and the multi-compositeness of the spectra of individual sugars complicate the improvement of protocols for control and identification of irradiated sugar-containing foodstuffs using EPR. A thorough understanding of the EPR spectrum of individual irradiated sugars hence seems a requirement for reliably using them in dosimetric applications.

Recently, the dominant room temperature stable radicals in irradiated sucrose [2] and  $\beta$ -D-fructose [3] have been thoroughly characterized in our lab using EPR, electron nuclear double resonance (ENDOR) and ENDOR-induced EPR. In this contribution we use the g and proton hyperfine interaction tensors obtained in these studies to simulate powder EPR spectra at the standard X-band (9.5 GHz), commonly used in applications, and at Q-band (34 GHz), rendering spectra with higher resolution. Simulations indicate that the major part of the dosimetric spectrum can be understood as arising from these dominant radicals, but that certain spectral components are still lacking in the simulations.

1. M. Ikeya, "New applications of electron spin resonance", World Scientific Publishing (1993), ISBN 981-02-1199-6.
2. H. De Cooman, E. Pauwels, H. Vrielinck, E. Sagstuen, S. Van Doorslaer, F. Callens, and M. Waroquier, *Phys. Chem. Chem. Phys.* 2009, **11**, 1105-1114, and references therein.
3. M. A. Tarpan, H. Vrielinck, H. De Cooman, and F. Callens, *J. Phys. Chem. A* 2009, **113**, 7994-8000, and references therein.